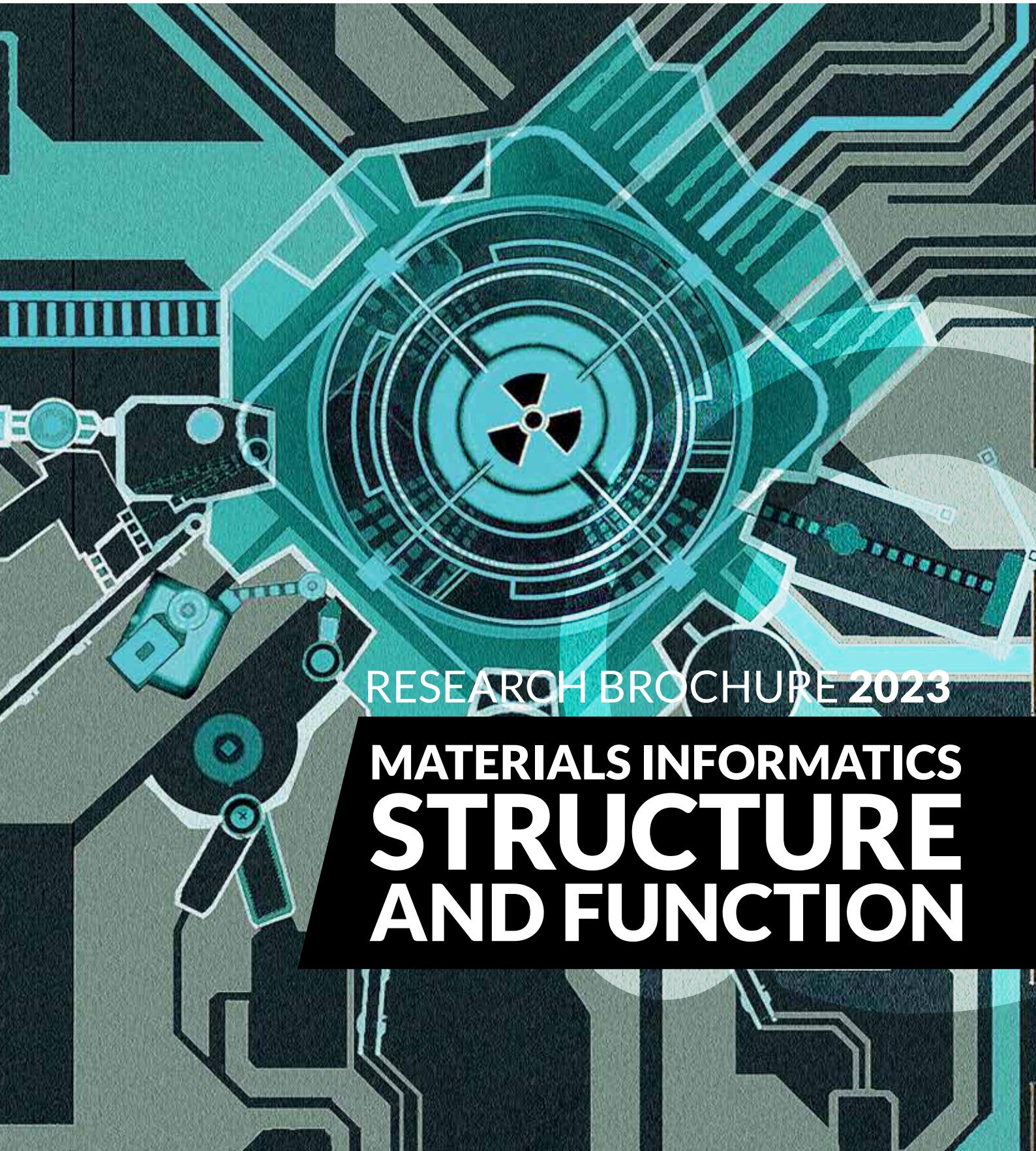
NOMATEN

Centre of Excellence in Multifunctional Materials
for Industrial and Medical Applications



RESEARCH BROCHURE **2023**

MATERIALS INFORMATICS STRUCTURE AND FUNCTION

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GENERAL SUMMARY BY PROF. STEFANOS PAPANIKOLAOU

RESEARCH GROUP LEADER: MATERIALS INFORMATICS, STRUCTURE AND FUNCTION

The Materials Informatics, Structure and Function (MASIF) group was established in late 2020 and represents the leading materials informatics research hub in NCBJ, Poland and Eastern Europe. Papanikolaou leads the MASIF group at the NOMATEN CoE. He is Associate Editor in the Springer-Nature open-access journal Materials Theory, as well as the Frontiers in Physics-Condensed Matter Physics. He has 70+ peer-reviewed publications, including more than 10 in machine learning aspects of materials science, with 1800+ total citations, and publications in high impact journals such as Nature, Nature Physics, Materials&Design, npj Comput. Materials.
The MASIF group is currently composed of 5 doctoral students, 3 postdoctoral associates (one of which is K. Frydrych) and technical staff members. Papanikolaou is currently writing a book on Materials Informatics Methods and Applications, towards future graduate students in Materials Science and Engineering programs. Finally, professional service and recognition has been evidenced through organizing more than 15 symposia in major conferences, being involved in the leadership of major regional (ASEE-NCS) and national (MRS) societies, and being on the editorial board of three peer-reviewed journals (Mat.Theory, J. Mechanics, Frontiers in Physics).

In the period 2020-2022, the MASIF Group has been established, starting from literally ashes, in September 2020, to a large group of 5 doctoral students, 3 postdoctoral associates, and 2 brilliant machine learning experts. The MASIF group has been publishing more than 10 manuscripts per year, has established high impact, strategic collaborations with top worldwide institutions (Harvard, MIT) and is on the verge of acquiring independent funding for establishing its sustainability.

The MASIF group, with the unwavering support of the NOMATEN CoE, has transitioned gradually and systematically, into a leadership position for Materials Informatics research. The culmination of such leadership was the organization and chairing of the very first Materials Informatics conference in Poland, at the NOMATEN premises in Swierk, during June 2022, with keynote visiting speakers, coming from top institutions in Poland, Italy, France, Finland, and USA. The conference was regarded as a success both for NCBJ (first ever on-site international conference), as well as NOMATEN and Poland, with major partnerships and collaborations established during and after the conference.

The MASIF group has been working systematically on the development of novel, state-of-art multiscale modeling approaches, as well as machine learning

methods and applications, for advanced materials, that are destined to be applicable in extreme conditions, such as high temperature and irradiation. The ultimate result of MASIF's systematic work has been the publication of 15 NOMATEN-produced manuscripts since Papanikolaou arrived at Swierk, and the submission of more than 30 manuscripts in total for publication in peer-reviewed, high-impact (>2.5) journals. The MASIF group is currently at its full capacity, with 5 doctoral students (Aligayev, Mammadli, Massa, Naghdi, Poisvert) and 3 postdoctoral associates (Karimi, Frydrych, Xu), as well as the support of 2 machine learning experts, with computer science degrees (Cieslinski, Tomczak). Finally, it is worth mentioning that currently the MASIF group has been accelerating its efforts, with multiple high-impact publications, collaborations, and project proposals being completed.

The MASIF group has concentrated its focus on **four major research avenues** that are keys for the development and excellence of NOMATEN:

- **Modeling of nanoindentation for advanced alloys**, using state-of-art strategies and machine learning. This is just one possible nanomechanics tool, but it is one that a colleague (Kurpaska) has been making strides in using it for high temperatures and advanced, multicomponent alloys such as high entropy alloys.

- **Development of machine learning interatomic potentials** (MLIP) for multiscale modeling applications, especially for nanomechanics. MLIPs are essential for multiscale modeling of advanced alloys and the MASIF group is taking a major leading position in Poland and Europe.

- **Materials design by using machine learning methods**, especially for „alloying" applications. Currently, the focus has been on hydrogen-related projects, due to the apparent societal impact of this work. However, the methods being developed are very general, and they will guarantee the sustainability of the MASIF group in the long-term. A key example of the sustainability path, is that MASIF was invited to co-author a M-ERA-NET project, led by major EU stakeholders, for hydrogen energy research.

- **Web-app and software development**, for materials informatics purposes, and targeted on materials science experimentalists.

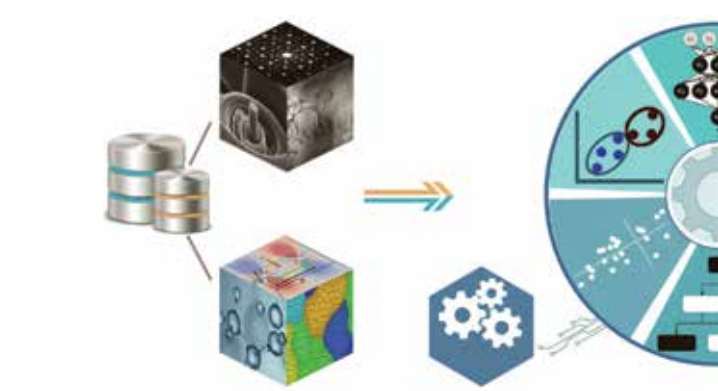
SCIENTIFIC DEVELOPMENTS

1. Modeling of nanoindentation for advanced alloys:

The MASIF group has focused on performing state-of-art predictions for mechanical properties, such as hardness and elastic moduli, as well as microstructural properties such as short-range order, segregation, in advanced multicomponent alloys. For this purpose, the group has been:

- Developing the first machine learning interatomic potential for nanomechanical applications, in an international collaboration, with particular focus on nanoindentation of single-crystalline molybdenum.

Figure: *AI wheel illustrating the tools and methods engaged in materials informatics:*



- Predicting that dwelling effects in nanoindentation can cause segregation phenomena in various equiatomic concentrated alloys.
- Collaborating with NOMATEN experimenters (Kurpaszka, Jozwik) towards machine learning automation of feature detection in nanoindentation maps of polycrystalline metal surfaces.
- Facilitating the interpretation of experimental nanoindentation datasets, by performing dedicated simulations, especially in the complex case of irradiated metal surfaces.

2. Development of machine learning interatomic potentials (MLIP):

The MASIF group is developing interatomic

potentials, with machine learning methods, for a variety of multicomponent advanced materials, especially focused on high entropy alloys, and irradiation applications. This work is being performed in collaboration with Harvard University, Massachusetts Institute of Technology, and CEA. The primary focus has been the identification of segregation effects and chemical kinetic mechanisms, especially in the proximity of grain boundaries.

3. Materials design by using machine learning methods,

The MASIF group is using machine learning tools towards the elucidation of design rules in metallurgy, based on fundamental ab-initio data and insights. Particular focus is being placed on „alloying" applications, either substitutional or interstitial. The MASIF group routinely scans through the periodic table for the identification of ideal alloying elements for particular applications.

Currently, the focus has been on hydrogen-related projects, due to the apparent societal impact of this work, especially for hydrogen energy production and storage. The methods being developed are general.

In particular,

a. Crystal graph neural networks and online databases have been utilized towards the identification of alloying effects in metals.

b. Density functional theory calculations have been performed for a variety of hydrogen-infused metals and hydrites, for identification of ideal microstructures.

c. Graphene-based defect structures have been investigated for catalyst applications in carbon reduction and hydrogen production projects.

4. **Web-app and software development:**

- The MASIF group has been developing the Materials Informatics software, MaterialsInformatics is a Python package that provides direct, easy-to-use black-box solutions for materials informatics applications, especially ones based on imaging data that emerge in materials science. https://github.com/MaterialInformatics/MaterialsInfomatics, https://pypi.org/project/MaterialsInformatics/, https://materialsinformatics.carrd.co/
- The MASIF group has been developing a search engine for nuclear-research-related images and information, that will be openly available to the world research community.
- The MASIF group has been developing an SEM image-based recognition software of irradiation-related features and defects.
- The MASIF group has been routinely promoting data accessibility on the web, through online databases and github-based available software and routines, for the advancement of materials science, and multiscale materials modeling.

Figure: CIŚ Computer Cluster HQ at NCBJ. Supercomputer at NCBJ supports MASIF group

SELECTED PAPERS ABSTRACTS

Materials informatics for mechanical deformation: A review of applications and challenges

Materials 2021, 14(19), 5764;
https://doi.org/10.3390/ma14195764

In the design and development of novel materials that have excellent mechanical properties, classification and regression methods have been diversely used across mechanical deformation simulations or experiments. The use of materials informatics methods on large data that originate in experiments or/and multiscale modeling simulations may accelerate materials' discovery or develop new understanding of materials' behavior. In this fast-growing field, we focus on reviewing advances at the intersection of data science with mechanical deformation simulations and experiments, with a particular focus on studies of metals and alloys. We discuss examples of applications, as well as identify challenges and prospects.

Unambiguous Identification of Crystal Plasticity Parameters from Spherical Indentation

Crystals 2022, 12(10), 1341;
https://doi.org/10.3390/cryst12101341

Identification of elastic and plastic properties of materials from indentation tests received considerable attention in the open literature. However, unambiguous and automatic determination of parameters in the case of the crystal plasticity (CP) model is still an unsolved problem. In this paper, we investigate the possibility to unambiguously identify the CP parameters from spherical indentation tests using finite element method simulations combined with evolutionary algorithm (EA). To this aim, we check the efficiency and accuracy of EA while fitting either load–penetration curves, surface topographies, or both at the same time. By fitting the results against simulation data with known parameters, we can verify the accuracy of each parameter independently. We conclude that the best option is to fit both load–penetration curve and surface topography at the same time. To understand why a given fitting scheme leads to correct values for some parameters and incorrect values for others, a sensitivity analysis was performed.

Shear banding instability in multicomponent metallic glasses: Interplay of composition and short-range order

SPhys. Rev. B 105, 094117 (2022),
https://doi.org/10.1103/PhysRevB.105.094117

The shear-banding instability in quasistatically driven bulk metallic glasses emerges from collective dynamics, mediated by shear transformation zones and associated nonlocal elastic interactions. It is also phenomenologically known that sharp structural features of shear bands are typically correlated to the sharpness of the plastic yielding transition, being predominant in commonly studied alloys composed of multiple different elements, that have very different atomic radii. However, in the opposite limit where elements' radii are relatively similar, plastic yielding of bulk metallic glasses is highly dependent on compositional and ordering features. In particular, a known mechanism at play involves the formation of short-range order dominated by icosahedra-based clusters. Here, we report on atomistic simulations of multicomponent metallic glasses with different chemical compositions showing that the degree of strain localization is largely controlled by the interplay between composition-driven icosahedra-ordering and collectively-driven shear transformation zones. By altering compositions, strain localization ranges from diffuse homogenized patterns to singular crack-like features. We quantify the dynamical yielding transition by measuring the atoms' susceptibility to plastic rearrangements, strongly correlated to the local atomic structure. We find that the abundance of short-range ordering of icosahedra within rearranging zones increases glassy materials' capacity to delocalize strain. This could be understood on the basis of structural heterogeneities that are enhanced by the presence of local order. The kind of plastic yielding can be often qualitatively inferred by the commonly used compositional descriptor that characterizes element associations, the misfit parameter δa, and also by uncommon ones, such as shear-band width and shear-band dynamics' correlation parameters.

Figure: The MASIF group has been developing the Materials Informatics software. MaTi MaterialsInformatics is a Python package that provides direct, easy-to-use black-box solutions for materials informatics applications, especially ones based on imaging data that emerge in materials science

FUTURE PLANS

The group's plan for the 2022-2024 period, is to accelerate in well-established avenues that are set up in the last two years: Submit more than 15 manuscripts/ year, publish very high impact manuscripts (Physical Review Letters, Nature Communications, etc.), get proposals funded and new projects started, publish web apps and contribute to online databases, provide support to experimental EU and NOMATEN labs, network with high-performing researchers in Poland and the EU. All these visionary tasks are currently in schedule and shall be reported in the next period with further details.

The MASIF group has been developing a Materials Informatics software that aims to promote machine learning solutions for experimenters in metallurgy and materials science. The software, labeled as MATI, has been under reconstruction by Maciej Tomczak, towards optimization of its design and development of web apps, and has been a key link for collaboration with other CoE groups (Jozwik, Kurpaska, Alava), towards the application of machine learning tools in materials science.

The MASIF group has 5 PhD graduate students that are currently in their 1st year of research project, and will become experts in materials informatics, machine learning, multiscale modeling and data science. All PhD students are performing systematic research and publish their results routinely, with more than 2 manuscripts per year on average, per researcher. The key in PhD research, however, is the pursuit of high impact -- and that's exactly the purpose of each individual's effort at MASIF.

The PhD students in MASIF are focused on aspects of the four major research avenues: Axel Poisvert is focused on multiscale modeling of advanced multicomponent alloys, Dario Massa is focused on material design, using ab initio methods, and informatics approaches for optimizing alloying combinations in advanced materials (in collaboration with E. Kaxiras at Harvard University), Amirhossein Naghdi is focused on the development of machine learning interatomic potentials for W, Mo and equiatomic NiCoCr (in collaboration with B. Kozinsky and E. Kaxiras at Harvard University and also, C. Marinica at CEA-Saclay), Amil Aligayev is focused on materials design using time-dependent Ab Initio methods and materials informatics approaches (in collaboration with Ju Li at MIT), and Bakhtiyar Mammadli is focused on machine learning and software development for micromechanics applications (in collaboration with M. Alava).

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